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13. ABSTRACT (Maximum 200 words)

This project has concentrated almost entirely on non-convex minimization problems in nonlinear elasticity theory and the existence of deformation-induced microstructure under severe loading conditions. As the microstructure develops and becomes more dense with increasing loads, the material weakens and the body has a softer response. Our minimizing sequences predict this property.

To complement our theoretical development, a large scale FEM code was implemented on the CM-200 machine. This code has a high refinement capability which allows us to study those regions of the body where the fine phase mixture occurs and the strain field becomes extremely irregular.

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Final Report
Grant: DAAL03-91-G-0184
Some Problems in the Mechanics of Solids
with Phase Mixtures

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18 February 1993

0.1 Abstract of Research Supported.

For the most part, the work of this project has concentrated on non-convex minimization problems in nonlinear elasticity theory, and the existence of deformation-induced microstructure under severe loading conditions. The following papers have been completed with the acknowledgement of the grant DAAL03-91-G-0184:

- [1] Fosdick, R.L. & Y. Zhang. The torsion problem for a nonconvex stored energy function. Accepted for publication. *Arch. for Rational Mech. Anal.*(1992).
- [2] Dunn, J.E. & Roger Fosdick. The Weierstrass condition for a special class of elastic materials. Accepted for publication. *J. Elasticity*(1992).
- [3] Fosdick, R.L. & Y. Zhang. Coexistent phase mixtures in the anti-plane shear of an elastic tube. Submitted for publication. *ZAMP*(1993).

In addition, some resources of this grant were used to help support the Ph.D. candidate J.H. Yu, whom I have advised, during the course of his thesis research. This work is not yet completed but it will be finished by June 1993, and Mr. Yu is expected to be awarded a Ph.D. degree. The thesis title is:

- [4] Yu, Jang-Horng. The Nonlinear Oscillation of Viscoelastic Cylindrical and Spherical Shells, 1993.

0.2 Report on [1].

Motivation for this work is contained in the interesting fundamental experimental observations of Bader and Nadai(1927), Takenaka(1928), and Nakanishi(1928) concerning the torsional deformation of steel bars. Some pictures of these observations, taken from a classic book of Nadai(1950) on the flow and fracture of solids are contained in the figures at the end of this report. These figures show that as the angle of twist is increased, the internal deformation pattern in a steel bar eventually undergoes a transition in which many small sliver-like zones of large shear occur. These zones are generally sector-shaped with a periodic circumferential distribution when viewed at in a right cross section. Sometimes the zones are seen to be wedge-shaped and distributed in the axial direction, in a longitudinal cross section of the bar. The experimental observations show that with increasing angle of twist the distribution of zones of large shear becomes more dense and that eventually the cross section of the bar contains essentially three regions of shear behavior: an inner core of classical torsion with small shear, an outer annular region of relatively large shear, and a mixture region in between, in which thin sector-shaped, or wedge-shaped zones of large shear are distributed periodically among zones of small shear.

In [1], we studied this phenomenon within the framework of minimization theory in nonlinear elasticity theory for a non-convex stored energy function, and in so doing we developed a new perspective on its origin. From an energetic point of view, the optimal deformed configuration of an elastic body is one which associates with the lowest total potential energy among all admissible states. Thus, if one considers the experimentally observed sector-shaped or the wedge-shaped zones of large shear as being of fundamental importance in establishing the optimal deformed configuration of highly twisted cylinders, then our goal was to provide a theoretical basis for why there exists a minimizing configuration for the total potential energy with such complicated microstructures.

Because the existence of zones of large shear distributed among the zones of small shear is evidence that there are two phases – large shear and small shear phases – in equilibrium coincidently, we adopted the idea that the stored energy function has a loss of local convexity in parts of its domain of definition. Then, in particular, we studied the non-convex minimization problem associated with the torsion of a solid incompressible, isotropic, and homogeneous elastic bar of fixed height and right circular cross section. We found that for an appropriate class of admissible deformations in the Sobolev space $W^{1,p}$, where $p > 2$, the classical equilibrium deformation field is a minimizer of the potential energy when the applied angle of twist is either sufficiently small or sufficiently large. However, for a broad range of moderate twists we found that there is no minimizer, and for these cases we construct a minimizing sequence which converges in a weak measure-theoretic sense to the infimum of the potential energy. This limiting sequence exhibits an infinitely fine microstructure analogous to a two-phase mixture of large and small states of shear. The volume fraction of large to small shear is found to depend on the radial position in the cross-section,

with the greater fraction of large shear being at the outer radius and decreasing with the radial position to zero at a particular radius determined by the material and the overall angle of twist. The general picture of our construction is much like the above experimental observations; an annular ring carries a dense radial dependent mixture of two-phase shears which changes continuously, at a determined radius, into a classical small shear, single-phase inner core. The radius of the inner core decreases as the angle of twist increases. We found that as the microstructure develops and becomes more dense with increasing angle of twist, the material is weakened and the torsional moment response becomes softer.

0.3 Report on [2].

A nonlinear hyperelastic material is characterized by a stored energy function $W(\cdot) : \mathcal{D} \rightarrow \mathbb{R}$, where \mathcal{D} is an open subset of the set of second order tensors on \mathbb{R}^3 with positive determinant. It is required that $W(\cdot)$ be *frame indifferent* or *objective*, i.e.,

$$W(QF) = W(F) \quad (1)$$

for all $F \in \mathcal{D}$ and for all proper, orthogonal tensors Q . Since (1) requires that $Q\mathcal{D} \subseteq \mathcal{D}$, objectivity is a restriction on both $W(\cdot)$ and its domain \mathcal{D} . We assume that $W(\cdot)$ is twice continuously differentiable on \mathcal{D} .

Let Ω be an open, bounded, and connected region of \mathbb{R}^3 with boundary $\partial\Omega$. Let $y^*(\cdot) : \partial\Omega \rightarrow \mathbb{R}^3$ be pre-assigned and consider the set \mathfrak{F} of one-to-one functions $y(\cdot) : \Omega \rightarrow \mathbb{R}^3$ which are continuous, piecewise smooth, meet $\nabla y(\Omega) \subseteq \mathcal{D}$, and have a continuous extension which agrees with the boundary data $y^*(\cdot)$ on $\partial\Omega$. In nonlinear elasticity theory a fundamental role is played by functions $\hat{y}(\cdot) \in \mathfrak{F}$ which

$$\text{minimize } \int_{\Omega} W(\nabla y) dv \text{ on } \mathfrak{F}. \quad (2)$$

As is well-known, wherever such minimizers $\hat{y}(\cdot)$ are sufficiently smooth, it is necessary that the *Weierstrass condition*

$$W(\nabla \hat{y}(x)) + (F - \nabla \hat{y}(x)) \cdot W_F(\nabla \hat{y}(x)) \leq W(F), \quad (3)$$

be satisfied for all $F \in \mathcal{D}$ such that $F - \nabla \hat{y}(x)$ is rank one.

Let us say that the function $W(\cdot) : \mathcal{D} \rightarrow \mathbb{R}$ is *rank 1 convex* at $\hat{F} \in \mathcal{D}$ if

$$W(\hat{F}) + (F - \hat{F}) \cdot W_F(\hat{F}) \leq W(F) \quad (4)$$

for all F such that $F - \hat{F}$ is rank 1. Also, let $\mathcal{D}^1 \subseteq \mathcal{D}$ denote the set of tensors at which $W(\cdot)$ is rank 1 convex. From (3), we see that the gradient of a minimizing field $\hat{y}(\cdot)$ must meet $\nabla \hat{y}(\Omega) \subseteq \mathcal{D}^1$, and, because of this, it is common to expect non-smooth minimizing fields whenever \mathcal{D}^1 is not connected.

With few exceptions, the implications of rank 1 convexity and the structure of \mathcal{D}^1 remain important open problems that require working through. In [2], we present necessary and sufficient conditions for $W(\cdot)$ to be rank 1 convex at a point $\hat{\mathbf{F}} \in \mathcal{D}$ for the special class of isotropic elastic materials for which

$$W(\mathbf{F}) = \psi(I), \quad (5)$$

where $I = |\mathbf{F}|^2$. We assume that $\psi(\cdot) : \mathcal{I} \rightarrow \mathbb{R}$ is twice continuously differentiable on $\mathcal{I} \equiv \{I | I = |\mathbf{F}|^2, \mathbf{F} \in \mathcal{D}\}$.

As a main result of this work, we prove the following theorem and study its consequences:

Theorem. *Suppose (5) holds. For $\hat{\mathbf{F}} \in \mathcal{D}$, set $\hat{\mathbf{B}} \equiv \hat{\mathbf{F}}\hat{\mathbf{F}}^T$, $\hat{I} \equiv \text{tr}(\hat{\mathbf{B}}) = |\hat{\mathbf{F}}|^2$, and let $\hat{\beta}_{\max}$ denote the maximum eigenvalue of $\hat{\mathbf{B}}$. Then, the stored energy function $W(\cdot) : \mathcal{D} \rightarrow \mathbb{R}$ is rank 1 convex at $\hat{\mathbf{F}} \in \mathcal{D}$ if and only if*

$$\psi'(\hat{I}) \geq 0, \quad (6)_1$$

and

$$\psi(\hat{I}) + 2\hat{\beta}_{\max} \left(\sqrt{1 + (I - \hat{I})/\hat{\beta}_{\max}} - 1 \right) \psi'(\hat{I}) \leq \psi(I) \quad (6)_2$$

for all $I \in \mathcal{I}$ such that $I \geq \hat{I} - \hat{\beta}_{\max}$.

Although the materials that we analyze here are too special to be of general applicability, they reveal clearly that subtle but important consequences flow from both the structure of \mathcal{D} and the structure of \mathcal{D}^1 . In this work, we are motivated by elasticity theory, stability, and coexistent phase structures, and because of that we admit only deformations and their gradients that preserve orientation. When this essential physical requirement is not enforced the results can be fundamentally different from those of (6), as is evidenced by the conclusions of Theorem 1.10 in Dacorogna's impressive 1989 book on the calculus of variations.

0.4 Report on [3].

In [3], we have studied the regularity properties of a solution to an anti-plane shear non-convex minimization problem and determined the existence and general nature of those sub-regions of the body (bordered by free boundaries which must be found as part of the solution) in which the strain field is expected to be highly irregular. In general, the problem has no minimizer but we construct a weakly convergent minimizing sequence of deformations in a certain Sobolev space for which the total potential energy converges to its infimum. We show that the minimizing sequence has a weak convergence property in a measure-theoretic sense, and we characterize the regularity properties of this sequence.

More specifically, we consider an isotropic elastic tube whose cross section is a convex ring whose outer lateral boundary is fixed and whose inner lateral surface is given a uniform displacement along its axial direction. Plasticity theory is commonly employed in the study of problems that involve the damage of materials and the localization of deformation (i.e., shear bands). Here, however, we provide a new perspective on the understanding of the mechanisms of material damage and the localization of severe deformations from an energetic (minimization) point of view. The non-existence of a minimizer to our characterizing non-convex minimization problem for a certain range of prescribed axial displacement of the inner lateral surface implies that among all "admissible" deformations there is none for which the values of the stored energy function correspond to its convex points almost everywhere in the body. Because of this, we find that to reach the infimum the tube divides into three characteristic subdomains—one of high strain, one of low strain, and one of intermediate "mixed" strain. In the intermediate "mixed" strain subdomain, the stored energy function loses its strict convexity. The main variational problem then gives rise to a free boundary value problem in which the subdomain where the strict convexity of the stored energy function breaks down must be determined as part of the solution. The description of this intermediate phase mixture region was one of the goals of this work. Generally, we find that it is a thin localized region through which the shear strain suffers a large change. This suggests the idea of a *shear band*—an idea more commonly encountered in studies involving classical plasticity theory.

As a complement to our theoretical development, we implemented an FEM code, developed originally for the Cray with a direct solver, and revised it so as to be compatible with the Connection Machine parallel environment and a GMRES iteration scheme. This code has a large refinement capability which allows us to study those regions of the body where the strain field is rapidly varying and becoming highly irregular, i.e., the part of the body which supports a fine phase mixture. Our numerical results on the CM-200 have established some interesting global features of the shape of the boundary of these important regions (free boundaries) that have so far alluded mathematical study. They also have confirmed much of our theoretical analysis of this problem. The fine phase mixture regions have the appearance of shear bands, and they are responsible for the dramatic softening response of the body as the loads are increased. Several additional exploratory numerical results are reported in [3] for this problem concerning bodies of various geometric cross sections and materials with stored energy functions having different nonconvexities. As an extension of both [1] and [3], we have begun to investigate the consequences of incorporating regularizing higher strain gradient terms into the constitutive equation so as to penalize the emergence of phase mixture zones and transition layers of rapid strain variation.

0.5 Report on [4].

In this thesis, Mr. Yu has studied the relationship between differential type and history type constitutive equations for describing the nonlinear behavior of solids. While the fading memory approximation to history functionals for retarded motions is known to lead to differential type constitutive relations, often this is assumed to imply that the solution of equivalent problems for the two constitutive theories will be "close" to one another in some reasonable sense. But, this is not generally true. A part of this dissertation is concerned with this issue within the context of the non-linear motion of solid viscoelastic cylindrical and spherical shells. The fundamental balance laws for this work are of two kinds—second order nonlinear ordinary differential equations, and second order nonlinear ordinary functional integral-differential equations of the delay type (highly non-standard). The elastic contribution to these equations is generally due to a non-convex strain energy function which carries with it the possibility of multiple equilibrium states, and this considerably complicates the story. In this case, chaotic-like motions have been determined.

The fading memory approximation for retarded motions has played an important part in the development of constitutive theory in continuum mechanics since the early 1960's, but its practical consequences are far from understood. In fact, since only constitutive theory is invoked in this approximation, it is not clear that adopting this procedure is at all reasonable if *approximate solutions of the equations of motion* are what one is after. A study such as that undertaken in [4] has a significant bearing on the development of approximation theory for the solution of problems in non-linear continuum mechanics.

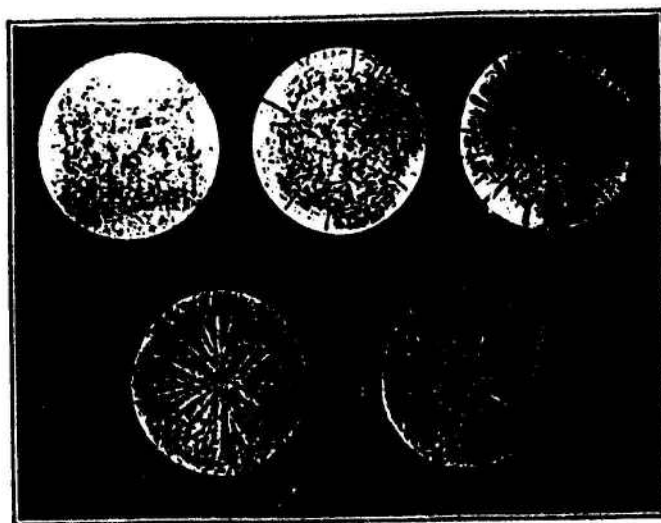


Figure 1: Cross sections of soft-iron bars of circular cross section subjected to a torsion deformation.

- a. $\frac{\theta}{H} = 0.007 \text{ deg/cm.}$ b. $\frac{\theta}{H} = 0.04 \text{ deg/cm.}$ c. $\frac{\theta}{H} = 0.22 \text{ deg/cm.}$
d. $\frac{\theta}{H} = 1.84 \text{ deg/cm.}$ e. $\frac{\theta}{H} = 3.02 \text{ deg/cm.}$

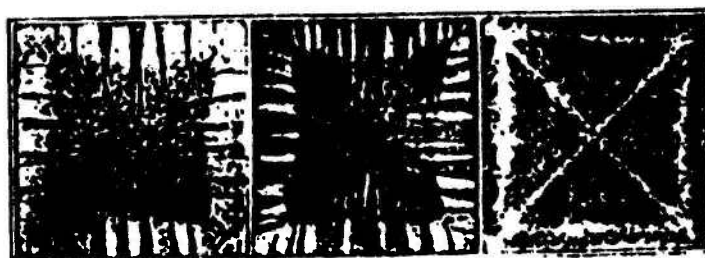


Figure 2: Cross sections of soft-iron bars with a square cross section subjected to a torsion deformation.

- a. $\frac{\theta}{H} = 0.38 \text{ deg/cm.}$ b. $\frac{\theta}{H} = 0.68 \text{ deg/cm.}$ c. $\frac{\theta}{H} = 0.90 \text{ deg/cm.}$

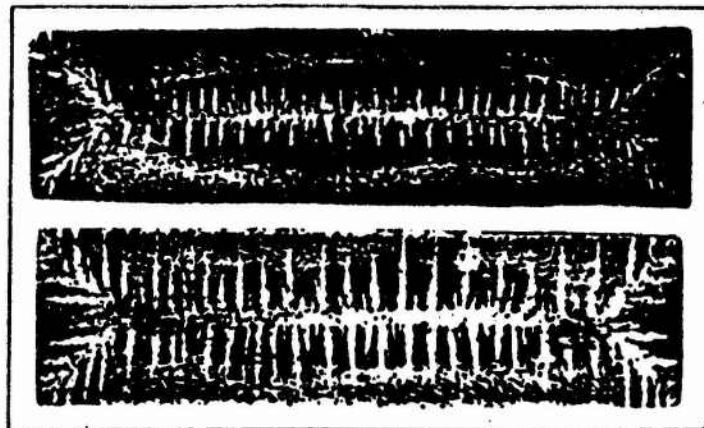
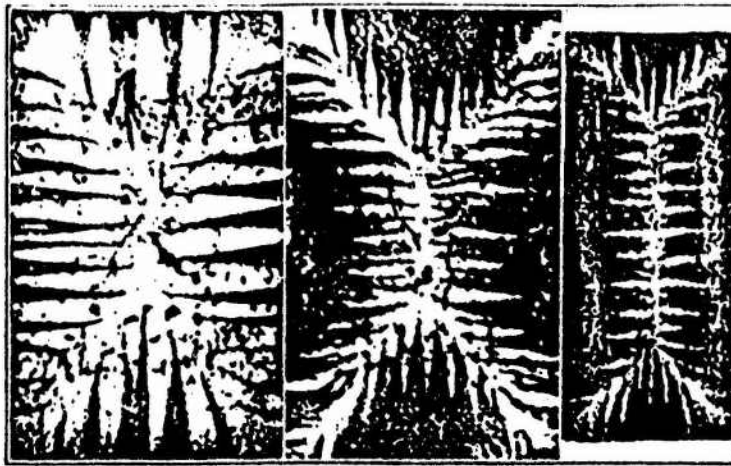


Figure 3: Cross sections of soft-iron bars with a rectangular cross section subjected to a torsion deformation.

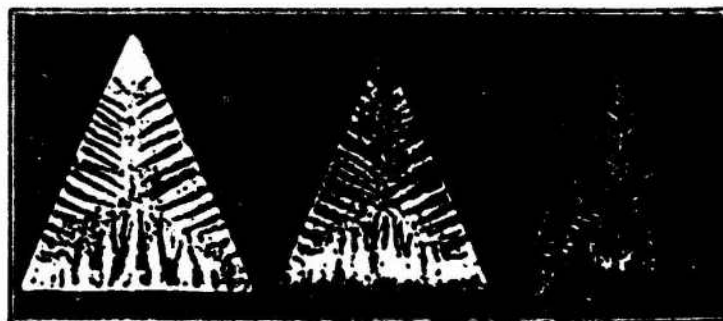


Figure 4: Cross sections of soft-iron bars with a triangular cross section subjected to a torsion deformation.